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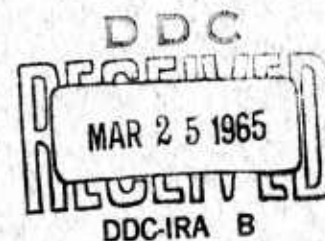
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A SUCCESSIVE SWEEP METHOD FOR SOLVING OPTIMAL PROGRAMMING PROBLEMS



By
Stephen R. McReynolds and Arthur E. Bryson, Jr.

March 2, 1965

Technical Report No. 463

Cruft Laboratory
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ABSTRACT

An automatic, finite-step numerical procedure is described for finding exact solutions to non-linear optimal programming problems. The procedure represents a unification and extension of the steepest-descent, and second variation techniques.

The procedure requires the backward integration of the usual adjoint-vector differential equations plus certain matrix differential equations. These integrations correspond, in the ordinary calculus, to finding the first and second derivatives of the performance index respectively. The matrix equations arise from an inhomogeneous Riccati transformation, which generates a linear "feedback control law" that preserves the gradient histories, $H_u(t)$, on the next step or permits changing them by controlled amounts, while also changing terminal conditions by controlled amounts. Thus, in a finite number of steps, the gradient histories can be made identically zero, as required for optimality, and the terminal conditions satisfied exactly. One forward plus one backward sweep, correspond to one step in the Newton-Raphson technique for finding maxima and minima in the ordinary calculus.*

As by-products, the procedure produces (a) the functions needed to show that the program is, or is not, a local maximum (the generalized Jacobi test) and (b) the feedback gain programs for neighboring optimal paths to the same, or a slightly different, set of terminal conditions.

CLASS OF PROBLEMS TREATED

The method is applicable to a class of non-linear optimal programming problems where one wishes to determine control functions $u(t)$ in $t_0 \leq t \leq t_1$ so as to minimize (or maximize) a performance index of the form

$$J = \phi[x(t_1), t_1] + \int_{t_0}^{t_1} L[x(t), u(t), t] dt \quad (1)$$

subject to the constraints

$$\dot{x} = f[x(t), u(t), t] \quad x(t) \text{ is an } n\text{-component state vector} \quad (2)$$

$u(t)$ is an m -component control vector

$$x(t_0) = x_0 \quad (3)$$

$$\psi[x(t_1), t_1] = 0 \quad \psi \text{ is a } q\text{-component vector } (q \leq n) \quad (4)$$

A further restriction on the class of problems treated in this paper is that we assume $\frac{\partial^2 H}{\partial u^2}$ is a positive-definite (or negative-definite) matrix over

* This latter technique is reviewed briefly in the Appendix to this paper.

the whole interval $t_0 \leq t \leq t_1$ where H is the variational Hamiltonian introduced in the next section.

The final time, t_1 , may be given either explicitly or implicitly in Eqns. (4). For simplicity of presentation, we will first discuss the case where the final time t_1 is given explicitly.

CASE WHERE FINAL TIME IS GIVEN EXPLICITLY

In the usual manner we introduce the auxiliary scalar functions

$$H(\lambda, x, u, t) = L(x, u, t) + \lambda^T f(x, u, t) \quad (5)$$

$$\Phi(v, x, t) = \phi(x, t) + v^T \psi(x, t) \quad (6)$$

where $\lambda(t)$ is an n -component vector of influence functions and v is a q -component constant vector. We regard $u(t)$ as control functions and v as control parameters, and introduce a modified performance index \bar{J} where

$$\bar{J} = \Phi[v, x(t_1), t_1] + \int_{t_0}^{t_1} \{H[\lambda(t), x(t), u(t), t] - \lambda^T(t) \dot{x}\} dt \quad (7)$$

Note that when (2) and (4) are satisfied, (7) is identical with (1).

Necessary conditions for an extremal path are (e.g. see Ref. 1)

$$\dot{\lambda}^T = -H_x \quad (8)$$

$$0 = H_u \quad (9)$$

$$\lambda^T(t_1) = \Phi_x[v, x(t_1), t_1] \equiv (\phi_x + v^T \psi_x)_{t=t_1} \quad (10)$$

Suppose we arbitrarily choose some control functions $u(t)$ and some control parameters v , integrate Eqns. (2) forward with initial conditions (3), and Eqns. (8) backward with boundary conditions (10). In general, Eqns. (4) and (9) will not be satisfied. Now, consider a perturbation around this path:

$$\delta \dot{x} = f_x \delta x + f_u \delta u \quad (11)$$

$$\delta \dot{\lambda} = -H_{xx} \delta x - f_x^T \delta \lambda - H_{xu} \delta u \quad (12)$$

$$\delta H_u = H_{ux} \delta x + H_{uu} \delta u + f_u^T \delta \lambda \quad \text{specified} \quad (13)$$

$$\delta x(t_0) \quad \text{specified} \quad (14)$$

$$\delta \lambda(t_1) = [\phi_{xx} \delta x + \psi_x^T \delta v]_{t=t_1} \quad (15)$$

$$\delta \psi = [\psi_x \delta x]_{t=t_1} \quad \text{specified} \quad (16)$$

We may regard (11)-(16) as a linear,

inhomogeneous two-point boundary value problem that determines the functions $\delta x(t)$, $\delta \lambda(t)$, $\delta u(t)$, and the parameters dv in terms of specified functions $\delta H_u(t)$ and specified parameters $\delta x(t_0)$ and $\delta \psi$. This is very close to the viewpoint taken by Merriam (Ref. 2) and Kelley, Kopp, and Moyer (Ref. 3).

To solve this two-point boundary value problem we may solve (13) for $\delta u(t)$ in terms of $\delta x(t)$, $\delta \lambda(t)$, and $\delta H_u(t)$, provided $H_{uu}(t)$ is non-singular:

$$\delta u = -H_{uu}^{-1}[-\delta H_u + H_{ux}\delta x + f_u^T\delta \lambda] \quad (17)$$

and, upon substituting (17) into (11) and (12), we obtain

$$\dot{\delta x} = A\delta x + B\delta \lambda + v \quad (18)$$

$$\dot{\delta \lambda} = C\delta x - A^T\delta \lambda + w \quad (19)$$

where

$$A = f_x - f_u H_{uu}^{-1} H_{ux} \quad (20)$$

$$B = -f_u H_{uu}^{-1} f_u^T \quad (21)$$

$$C = -H_{xx} + H_{xu} H_{uu}^{-1} H_{ux} \quad (22)$$

$$v = f_u H_{uu}^{-1} \delta H_u \quad (23)$$

$$w = -H_{xu} H_{uu}^{-1} \delta H_u \quad (24)$$

THE INHOMOGENEOUS RICATTI TRANSFORMATION

In view of Eqns. (15) and (16), let us introduce the following inhomogeneous Ricatti transformation (suggested in Refs. 4, 5):

$$\delta \lambda(t) = P(t)\delta x(t) + R(t)dv + h(t) \quad (25)$$

$$\delta \psi = R^T(t)\delta x(t) + Q(t)dv + g(t) \quad (26)$$

where dv and $\delta \psi$ are constant infinitesimal vectors, $P(t)$, $R(t)$, and $Q(t)$ are matrix functions, and $h(t)$ and $g(t)$ are vector functions. Now, differentiate (17) and (18) with respect to time:

$$\dot{\delta \lambda} = P\dot{\delta x} + \dot{P}\delta x + \dot{R}dv + \dot{h} \quad (27)$$

$$0 = R^T\dot{\delta x} + \dot{R}^T\delta x + \dot{Q}dv + \dot{g} \quad (28)$$

Using (25) in (18) gives

$$\dot{\delta x} = (A+BP)\delta x + BRdv + Bh + v \quad (29)$$

Equating (19) and (27) and using (25) and (29) to eliminate $\dot{\delta x}$ and $\delta \lambda$, we have:

$$(C-A^T P-PA-PBP-\dot{P})\delta x - [(A^T+PB)R+\dot{R}]dv - [(A^T+PB)h+Pv-w+\dot{h}] = 0 \quad (30)$$

In a similar fashion, substitute (29) into (28):

$$[\dot{R}^T+R^T(A+BP)]\delta x + (R^T BR+\dot{Q})dv + R^T(Bh+v) + \dot{g} = 0 \quad (31)$$

Viewing (30) and (31) as identities, valid for arbitrary values of δx and dv , it follows that the coefficients of δx and dv must vanish; this yields differential equations for P , R , Q , h , and g . Also, if we require that (30) and (31) be equivalent to (15) and (16) at the terminal time, we

obtain boundary conditions for P , R , Q , h , and g :

$$\dot{P} = -A^T P - PA - PBP + C; P(t_1) = [\phi_{xx} \phi_{xx}^T + v \psi_{xx}^T]_{t=t_1} \quad (32)$$

$$\dot{R} = -(A^T+PB)R; R(t_1) = [\psi_x^T]_{t=t_1} \quad (33)$$

$$\dot{Q} = -R^T BR; Q(t_1) = 0 \quad (34)$$

$$\dot{h} = -(A^T+PB)h - Pv + w; h(t_1) = 0 \quad (35)$$

$$\dot{g} = R^T(Bh+v); g(t_1) = 0 \quad (36)$$

Note that (32) is a nonlinear matrix differential equation (a matrix Riccati equation), while (33) is a linear matrix differential equation using the solution of (32); (34) is a matrix quadrature using the solution of (33); (35) is a linear vector differential equation using the solution of (32), and (36) is a vector quadrature using the solution of (35).

By integrating (32)-(36) backward along with (8) from t_1 to t_0 (a "backward sweep") we generate all possible solutions to (11)-(13) that satisfy the terminal conditions (15)-(16). We may think of (25)-(26) as "boundary conditions" at time $t < t_1$ that are equivalent to the boundary conditions (15)-(16) at time $t = t_1$. Thus the boundary conditions at the terminal time are "swept" backward to the initial time; a "forward sweep" then generates the required particular solution that also satisfies the initial conditions (14). This is precisely the approach taken by Bryson and Frazier (Ref. 6) to solve the linear smoothing problem except that the sweeps occur in the opposite order; the "forward sweep" is the Kalman-Bucy filter which involves a matrix Riccati equation, and the "backward sweep" gives the smoothing solution that satisfies the terminal conditions.

After completing the backward sweep, the required values of dv in terms of the desired infinitesimal changes $\delta H_u(t)$, $\delta x(t_0)$, and $\delta \psi$ can be obtained using (26):

$$dv = [Q^{-1}(\delta \psi - g - R^T \delta x)]_{t=t_0} \quad (37)$$

Having these values of dv , we could, in principle, substitute them into (29) and integrate these equations forward with (25) and (17) to find $\delta x(t)$, $\delta \lambda(t)$, and $\delta u(t)$ (a "forward sweep").

Alternatively, using (25) we could regard (17) as a linear feedback law for determining $\delta u(t)$:

$$\delta u(t) = -H_{uu}^{-1}(t) \{ [H_{ux}(t) + f_u^T(t)P(t)]\delta x(t) + f_u^T(t)R(t)dv - \delta H_u(t) + f_u^T(t)g(t) \} \quad (38)$$

Note that dv in (38) may be evaluated at the initial time $t = t_0$ as was done in (37) or we may evaluate it at several intermediate times in the manner of a sampled-data feedback law or we may evaluate it continuously in the manner of a continuous feedback law. If we do evaluate dv continuously, then (38) becomes

$$\delta u(t) = -H_{uu}^{-1} \{ [H_{ux} + f_u^T(P-RQ^{-1}R^T)] \delta x + [f_u^T R Q^{-1}] \delta \psi + [-\delta H_u + f_u^T(h-RQ^{-1}g)] \} \quad (38a)$$

Now, the first term in square brackets on the right hand side of (38a) is a linear feedback on deviations $\delta x(t)$ from the nominal state variable histories and will keep $\delta H_u(t) = 0$, $\delta \psi = 0$, for $\delta x(t_0) \neq 0$.

The second term in square brackets is the forcing function necessary to produce the desired changes $\delta \psi$ while holding $\delta H_u(t) = 0$. The third term in square brackets is the forcing function necessary to produce the desired changes $\delta H_u(t)$ while holding $\delta \psi = 0$; it is a linear functional of $\delta H_u(t)$, and vanishes if $\delta H_u(t) = 0$. We could, therefore, integrate (2) forward (a "forward sweep"), using (38) in

$$u(t) = u_{old}(t) + \delta u(t) \quad (39)$$

$$\delta x(t) = x(t) - x_{old}(t) \quad (40)$$

The advantage of this procedure over previous gradient procedures is that we have separate, precise control over the desired changes $\delta H_u(t)$ and $\delta \psi$.

By repeating this forward-backward sweep several times we can bring $H_u(t)$ and $\psi[x(t_1), t_1]$ precisely to zero while increasing the performance index; the required number of steps depends on the successful range of linearization of (11)-(16). We suggest that if N steps are to be used, it would be reasonable to choose

$$\delta H_u(r)(t) = -\epsilon(r) H_u(r-1)(t) \quad (41)$$

$$\delta \psi(r) = -\epsilon(r) \psi(r-1)[x(t_1), t_1] \quad (42)$$

where $\epsilon(r) = r/N$ and r is the step number; in this way, larger and larger reductions in the "residuals" are taken each step and, on the last step, the whole remaining correction is made, bringing $H_u(t)$ and ψ precisely to zero.

LOCAL OPTIMALITY - GENERALIZED JACOBI TEST AND CONJUGATE POINTS

When we have succeeded in bringing $H_u(t) = 0$ and $\psi[x(t_1), t_1] = 0$, we have generated an admissible extremal path. For this case, the feedback law (38a) simplifies to:

$$\delta u(t) = -H_{uu}^{-1}(t) [H_{ux} + f_u^T(P-RQ^{-1}R^T)] \delta x(t) \quad (43)$$

since $\delta \psi = 0$ and $\delta H_u(t) = 0$ implies that $v = w = h = g = 0$ (see Eqns. (23), (24), (35), (36)). If the symmetric $m \times m$ matrix $H_{uu}(t)$ is positive (or negative) definite and the symmetric $n \times n$ matrix $P-RQ^{-1}R^T$ is finite over the semi-open interval $t_0 \leq t < t_1$, then (43) indicates $\delta u(t) = 0$ if $\delta x(t_0) = 0$ and we are assured that we have generated a path that is at least a local optimal path. This is a generalized Jacobi test; if $P-RQ^{-1}R^T$ becomes infinite at some point this

is called a conjugate point to the terminal manifold $\psi[x(t_1), t_1] = 0$. An extremal path is not an optimal path if it contains a conjugate point (see e.g. Ref. 4).

INTERPRETATION OF THE MATRICES P, Q, AND R

Let us define a return function, $V(v, u, x, t)$ which is the value of \bar{J} in (7) when starting from state x at time $t < t_1$ using the control

functions $u(t)$ in (2) and the control parameters v . Infinitesimal variations away from a given set of initial conditions, $\delta x(t)$, and infinitesimal changes in the control parameters, dv , while holding $\delta H_u(t) = 0$, will produce an infinitesimal change in the return function, δV , given by

$$\delta V = \begin{bmatrix} \lambda^T(t), \psi^T[x(t_1), t_1] \end{bmatrix} \begin{bmatrix} \delta x(t) \\ dv \end{bmatrix} + \frac{1}{2} \begin{bmatrix} \delta x^T(t), dv^T \end{bmatrix} \begin{bmatrix} P(t), R(t) \\ R^T(t), Q(t) \end{bmatrix} \begin{bmatrix} \delta x(t) \\ dv \end{bmatrix} \quad (44)$$

From (44) it is clear that

$$\lambda^T(t) = \frac{\partial V}{\partial x(t)}, \quad \psi^T = \frac{\partial V}{\partial v}, \quad (45)$$

$$P(t) = \frac{\partial^2 V}{\partial x(t) \partial x(t)}, \quad R = \frac{\partial^2 V}{\partial v \partial x(t)}, \quad Q = \frac{\partial^2 V}{\partial v^2}$$

From (26), or (45)-(46), we can also write

$$R^T(t) = \frac{\partial \psi}{\partial x(t)}, \quad Q(t) = \frac{\partial \psi}{\partial v} \quad (46)$$

and we note these quantities are similar to the steepest-ascent quantities $\lambda^{(\psi)}(t)$ and $I_{\psi\psi}(t)$ of Bryson and Denham (Ref. 7).

If the path is extremal ($H_u(t) = 0$), and satisfies the terminal conditions ($\psi[x(t_1), t_1] = 0$), then $V = V(x, t)$ is the optimal return function of Hamilton-Jacobi-Bellman theory (see e.g. Ref. 8). Equation (44), using (26) with $\delta \psi = 0$, $g = 0$, to eliminate dv becomes

$$\delta V = \lambda^T \delta x + \frac{1}{2} \delta x^T (P-RQ^{-1}R^T) \delta x \quad (47)$$

which gives the infinitesimal change in the optimal return function for infinitesimal changes in the initial conditions $\delta x(t)$ holding the final conditions constant ($\delta \psi = 0$).

SUMMARY FOR CASE WHERE FINAL TIME IS GIVEN EXPLICITLY

(A) Estimate the control functions $u(t)$ and integrate $\dot{x} = f(x, u, t)$ forward with given values of $x(t_0)$. Record the constants $\psi[x(t_1), t_1]$, and the functions $u(t)$, $x(t)$.

(B) Estimate the control parameters v and $\dot{\lambda} = -f_x^T \lambda$ backward with $\lambda(t_1) = [\phi_x + v^T \psi_x]_{t=t_1}$, integrate

using $u(t)$, $x(t)$ to evaluate $f_x[x(t), u(t), t]$. Calculate $H = \lambda^T f$ and its derivatives H_u , H_{uu} ,

H_{ux} , H_{xx} as you go. H_{uu}^{-1} must also be calculated. While doing so, one can verify that H_{uu} is positive (or negative) definite. If H_{uu} does not satisfy the appropriate condition, better estimates of $u(t)$ and v are required in (A).

(C) Simultaneously with (B), integrate Eqns. (32)-(36) for P , Q , R , h , and g backward, using the derivatives of H from (B) and $\delta H_u(t)$ from (41). Record the forcing functions

$$H_{uu}^{-1}(t)[- \delta H_u(t) + f_u^T(t)h(t)] = U(t)$$

and the feedback gains

$$H_{uu}^{-1}(t)[H_{ux}(t) + f_u^T(t)P(t)] = K(t)$$

$$H_{uu}^{-1}(t)f_u^T(t)R(t) = L(t)$$

(D) Determine and record the parameters dv from (37), i.e.

$$dv = Q^{-1}(t_0)[\delta \psi - g(t_0) - R^T(t_0)\delta x(t_0)]$$

(E) Repeat (A) using the improved estimates of $u(t)$

$$u(t) = u_{old}(t) + U(t) - K(t)[x(t) - x_{old}(t)] - L(t)dv$$

(F) Repeat (B), (C), and (D) using the improved estimates of u , v ,

$$v = v_{old} + dv$$

(G) Repeat (E) and (F) until $H_u(t) = 0$, $\psi[x(t_1), t_1] = 0$.

CASE WHERE FINAL TIME IS GIVEN IMPLICITLY

If the final time, t_1 , is given implicitly in (4), then it is necessary to estimate t_1 for the first forward sweep, in addition to $u(t)$ and v . A few additional equations must be integrated on the backward sweep in order to determine the required dt_1 for the next forward sweep.

The development is the same as in the previous case through Eqn. (10); at that point an additional necessary condition is required to determine the final time, namely the transversality condition

$$\Omega[x(t_1), t_1] = [\phi_t + \phi_x f + L]_{t=t_1} = 0 \quad (48)$$

The development is again the same up to Eqns. (15) and (16) which are replaced by the following:

$$\begin{bmatrix} \delta \lambda(t_1) \\ d\psi \\ d\Omega \end{bmatrix} = \begin{bmatrix} \phi_{xx}(t_1) & \psi_x^T(t_1) & m(t_1) \\ \psi_x(t_1) & 0 & n(t_1) \\ m^T(t_1) & n^T(t_1) & a(t_1) \end{bmatrix} \begin{bmatrix} \delta x(t_1) \\ dv \\ dt_1 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ H_{uu}^{-1} \delta H_u \end{bmatrix} \quad (49)$$

where

$$m^T(t_1) = [\Omega_x - H_{uu} H_{ux} (H_{ux} + f_u^T \phi_x)]_{t=t_1} \quad (52)$$

$$n^T(t_1) = \left[\frac{D\psi}{Dt} - H_{uu}^{-1} f_u^T \psi_x \right]_{t=t_1} \quad (53)$$

$$a(t_1) = \left[\frac{D}{Dt} \left(\frac{D\phi}{Dt} + L \right) \right]_{t=t_1} \quad (54)$$

and

$$\frac{D(\cdot)}{Dt} = \frac{\partial(\cdot)}{\partial t} + \frac{\partial(\cdot)}{\partial x} \dot{x} + \frac{\partial(\cdot)}{\partial u} \dot{u}$$

$$\dot{u} = -H_{uu}^{-1}(f_u^T \phi_x + H_{ux} + f_u^T \phi_x + H_{ux} f)$$

Equations (17)-(24) are still applicable but, in view of (49)-(51), the inhomogeneous Riccati transformation beginning at (25) must be generalized to the following:

$$\begin{bmatrix} \delta \lambda(t) \\ d\psi \\ d\Omega \end{bmatrix} = \begin{bmatrix} P(t) & R(t) & m(t) \\ R^T(t) & Q(t) & n(t) \\ m^T(t) & n^T(t) & a(t) \end{bmatrix} \begin{bmatrix} \delta x \\ dv \\ dt_1 \end{bmatrix} + \begin{bmatrix} h(t) \\ g(t) \\ \beta(t) \end{bmatrix} \quad (55)$$

$$d\psi = R^T(t)Q(t)dv + g(t) \quad (56)$$

$$d\Omega = m^T(t)n^T(t)dt_1 + \beta(t) \quad (57)$$

Differentiating (55)-(57) with respect to time, using the fact that $d\psi$, $d\Omega$, dv , and dt_1 are constants, we obtain

$$\begin{bmatrix} \delta \dot{\lambda} \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \dot{P} & \dot{R} & \dot{m} \\ \dot{R}^T & \dot{Q} & \dot{n} \\ \dot{m}^T & \dot{n}^T & \dot{a} \end{bmatrix} \begin{bmatrix} \delta x \\ dv \\ dt_1 \end{bmatrix} + \begin{bmatrix} \dot{P} \\ \dot{R}^T \\ \dot{m}^T \end{bmatrix} \begin{bmatrix} h \\ g \\ \beta \end{bmatrix} \quad (58)$$

$$0 = \dot{R}^T Q \dot{dv} + \dot{R}^T \dot{\delta x} + \dot{g} \quad (59)$$

$$0 = \dot{m}^T n^T \dot{dt_1} + \dot{m}^T \dot{\delta x} + \dot{\beta} \quad (60)$$

Using (55) in (18) gives

$$\delta \dot{x} = (A + BP)\delta x + BRdv + BMdt_1 + Bh + v \quad (61)$$

Using (55) in (19), together with (61), we can eliminate $d\dot{\lambda}$ and $\delta \dot{x}$ from (58)-(60), and obtain three equations like (30) and (31) in δx , dv , and dt_1 . These three equations are satisfied

identically if we choose P , Q , R , h , and g to satisfy (32)-(36) and m , n , a to satisfy

$$\dot{m} + (A^T + PB)m = 0 \quad (62)$$

$$\dot{n} = -R^T Bm \quad (63)$$

$$\dot{a} = -m^T Bm \quad (64)$$

$$\dot{\beta} = -m^T (Bh + v) \quad (65)$$

where the boundary conditions for m , n , a are given by (52)-(54). Note (62) is the same linear vector differential equation as (33) whereas (63) and (64) are simply quadratures.

If (62)-(65) are included in the backward integration sweep, then it is possible to solve for both dv and dt_1 at $t = t_0$, using (56) and (57) where desired values of $d\psi$ and $d\Omega$ for the next step are introduced. The desired value of $\delta H_u(t)$ must be used in solving for h , g , and β from (35), (36), and (64).

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APPENDIX

THE NEWTON-RAPHSON METHOD AND ITS APPLICATIONS TO ORDINARY CALCULUS PROBLEMS

In this Appendix the Newton-Raphson method is briefly stated. It will be seen that the Newton-Raphson method applied to optimization problems becomes a second-order iterative scheme which can be applied in the neighborhood of a non-singular optimum in order to obtain rapid convergence.

The formulation of second order steepest-ascent methods may be based upon a simple extension of the Newton-Raphson method used to solve a set of simultaneous nonlinear equations. Suppose one wishes to find an n -vector $x = (x_1, \dots, x_n)$ such that

$$P(x) = 0 \quad P = (P_1, \dots, P_n) \quad (A1)$$

The Newton-Raphson method generates a sequence $(x^{(0)}, x^{(1)}, \dots)$ by means of an iterative relation (A2).

$$x^{k+1} = x^k - \left[\left(\frac{\partial P}{\partial x} \right)^{-1} P \right]_{x=x^k} \quad (A2)$$

The rationale for this is obtained by expanding $P(x)$ in a power series around x^k .

$$P(x^k + dx) = P(x^k) + \frac{\partial P}{\partial x} \bigg|_{x=x^k} dx + O(dx^2) \quad (A3)$$

Setting $P(x^k + dx) = 0$, one sees that

$$dx = - \left(\frac{\partial P}{\partial x} \right)^{-1} P(x^k) + O(dx^2) \quad (A4)$$

By ignoring second and higher order terms on the right hand side of (A4) one obtains an estimate of the error in x within first order accuracy. Thus (A2) approximates the solution within a second order error. The method naturally assumes $\frac{\partial P}{\partial x}$ to be nonsingular in the region containing (x^k) and the solution.

The Newton-Raphson method may be extended to finding a local maximum of a function of several variables $f(x)$. If f is continuously differentiable, a local maximum x is characterized by being a solution to the following equations

$$f_{x_i} = 0 \quad i = 1, \dots, n \quad (A5)$$

Applying the Newton-Raphson method to these equations, one arrives at a second-order steepest-ascent method by merely identifying f_{x_i} with P_i in (A2).

The method may be readily extended to problems with constraints. Suppose the maximum of f is wanted subject to the added constraint

$$g(x) = 0 \quad (A6)$$

In place of this problem one may substitute the problem of extremizing $f + \lambda g$ with respect to x and λ as independent variables. This problem has no constraints and may be handled as the first case. An extremal is characterized by (A6) and

$$f_x + \lambda g_x = 0 \quad (A7)$$

Expanding (A6) around a nominal solution (x^k, λ^k) one obtains the following set of linear, inhomogeneous equations to solve:

$$0 = (f_x + \lambda g_x) \bigg|_{x^k, \lambda^k} + (f_{xx} + \lambda g_{xx}) dx + g_x d\lambda \quad (A8)$$

$$0 = g \bigg|_{x^k} + g_x dx$$

Solving (A8) yields corrections dx and $d\lambda$, and the second order steepest-ascent method becomes

$$x^{k+1} = x^k + dx \quad (A9)$$

$$\lambda^{k+1} = \lambda^k + d\lambda$$

Several cautions must be exercised. One is that dx must be small in order to guarantee convergence, which implies that the original error should not be too big. Secondly, the nominal and the maximum must be non-singular and normal. This is necessary to guarantee the inversion of the basic equations. The non-singularity condition guarantees that one can solve for dx . The normality condition guarantees that one can solve for $d\lambda$. Thirdly, one should note that the second-order steepest-ascent method seeks out stationary solutions, regardless of whether they are local minima, local maxima, or saddle points. In order to be sure that the sequence converges to the desired extremum, the eigenvalues of the second derivative matrix must be checked. This can be seen for the problem without constraints by substituting (A2) with $P = f_x$ into a power series for f around x^k .

$$f(x^{k+1}) = f(x^k) - \frac{1}{2} f_{xx}^{-1} f_x^2 + O(f_x^3) \quad (A10)$$

In order to guarantee that $f(x^{k+1}) > f(x^k)$, it is necessary to assume $f_{xx} < 0$.

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